

=>
Uploading C:\Program Files\Stnexp\Queries\10580610-secondary.str



chain nodes :
11 12 13 14 26 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 17 18 19 20 21 22 23 24 25
chain bonds :
8-11 9-12 12-13 12-14 24-26 26-27 26-28
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 17-18 17-22 18-19 19-20 20-21
21-22 21-23 22-25 23-24 24-25
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 8-11 9-12 12-13 12-14 17-18
17-22 18-19 19-20 20-21 21-22 21-23 22-25 23-24 24-25 24-26 26-27 26-28
isolated ring systems :
containing 1 : 17 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS
12:CLASS 13:CLASS 14:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:CLASS 27:CLASS 28:CLASS
fragments assigned reactant/reagent role:
containing 1
node mappings:
7:23 8:24 9:25 6:22 5:21 4:20 3:19 2:18 1:17

L1 STRUCTURE UPLOADED

=> s 11 sss full
FULL SEARCH INITIATED 08:49:12 FILE 'CASREACT'
SCREENING COMPLETE - 875 REACTIONS TO VERIFY FROM 92 DOCUMENTS

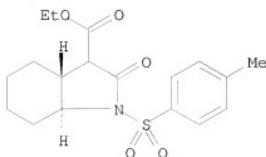
100.0% DONE 875 VERIFIED 6 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.04

L3 3 SEA SSS FUL L1 (6 REACTIONS)

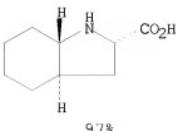
=> d 13 tot

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(22) OF 36 - 4 STEPS



1. NaCl, Water, DMF
2. AlH(Bu-i)2, CH2Cl2,
Hexane
3. Me3SiCN, SnCl4,
CH2Cl2
4. HCl, AcOH



REF: PCT Int. Appl., 2005054194, 16 Jun 2005

NOTE: 3) stereoselective

CON: STEP(1.1) room temperature -> 145 deg C; 140 - 145 deg C;
1.5 hours, 140 - 145 deg C; 18 hours, 140 - 145 deg C

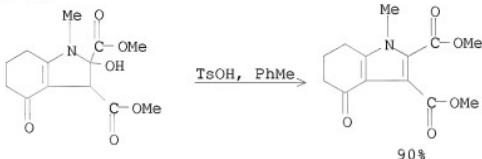
STEP(2) 50 minutes

STEP(3) 3 hours, -5 deg C

STEP(4.1) 1 hour, 100 deg C; 100 deg C; 19 hours, 100 deg C

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(29) OF 172



REF: European Journal of Organic Chemistry, (1), 190-208; 2003
CON: 1.5 hours, reflux

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(63) OF 508



REF: Helvetica Chimica Acta, 72(7), 1554-82; 1989